



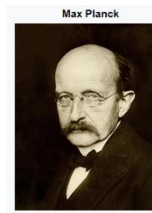
Schrödinger Wave Equation

Class - 1

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Louis de Broglie



Max Planck



Schrödinger's Cat is Dead



Erwin Schrödinger

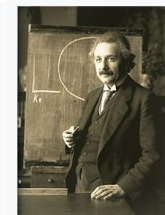


Max Born

$$\hat{H}\Psi(r,\theta,\Phi) = E\Psi(r,\theta,\Phi)$$



Niels Bohr



Albert Einstein



Schrödinger Wave Equation

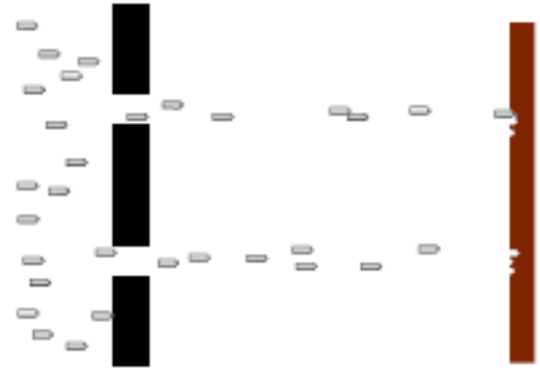
Erwin Schrödinger (1927) wrote an equation of motion for particles (like electrons) that account for their wave-like properties





Experiment with bullet

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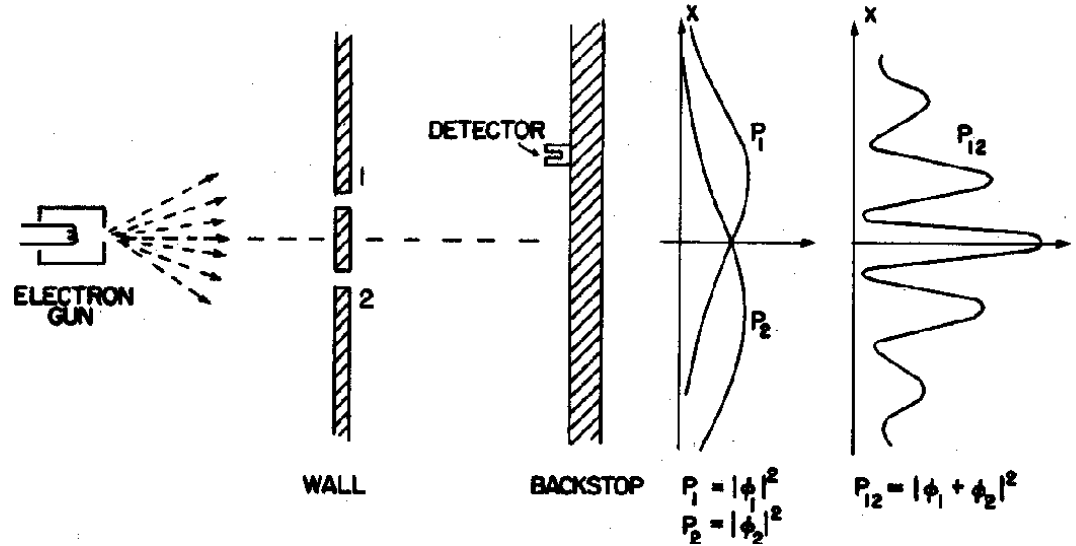


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Experiment with electrons

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Schrödinger Wave Equation

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Case 1:

When wavelength of a particle is the size of the our environment (**classical mechanics perfectly works**)

Case 2:

When wavelength of a particle is not according to size of the our environment (**classical mechanics fails**)





The Schrödinger equation is to quantum mechanics like Newton's equations of motion are to classical mechanics.

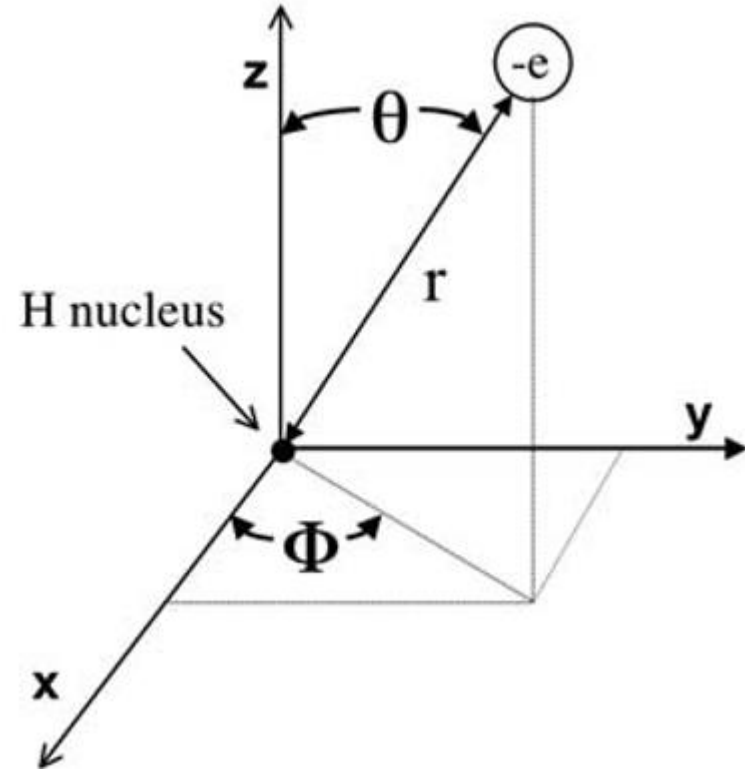
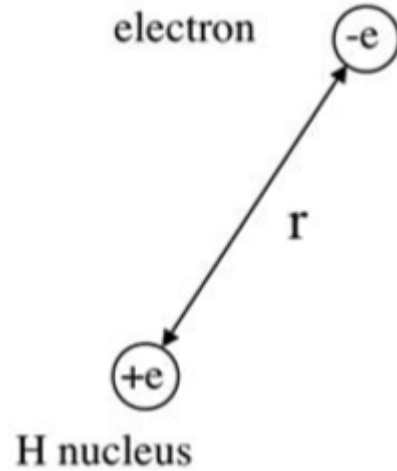




Schrödinger Wave Equation

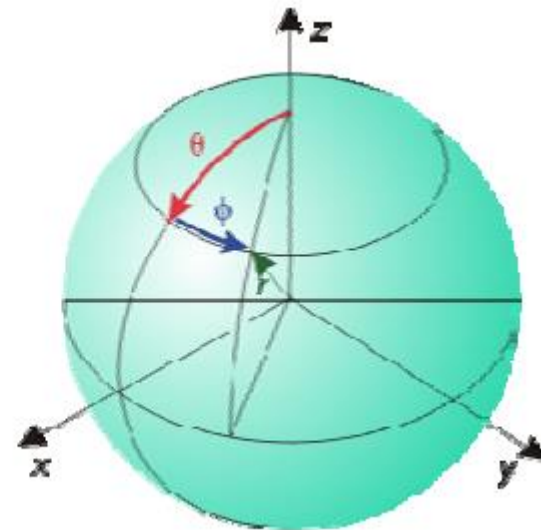
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$$\Psi_{(x)}(r, \theta, \phi)$$





$$\begin{aligned}x &= r \sin \theta \cos \phi \\y &= r \sin \theta \sin \phi \\z &= r \cos \theta\end{aligned}$$



$$\Psi_{(nlm)}(r, \theta, \phi) = R_{nl}(r) \underbrace{Y_{lm}(\theta, \phi)}_{\text{angular part}}$$

radial part





Schrödinger Wave Equation

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$$\Psi_{(x)} = 2a \cos \frac{2\pi x}{\lambda}$$



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Schrödinger Wave Equation

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$$\Psi_{(x)} = 2a \cos \frac{2\pi x}{\lambda}$$

How, $\Psi_{(x)}$ changes with time,
(take derivatives)

$$\Rightarrow \frac{d\Psi_{(x)}}{dx} = -2a \frac{2\pi}{\lambda} \cdot \sin \frac{2\pi x}{\lambda}$$





Schrödinger Wave Equation

$$\Psi_{(x)} = 2a \cos \frac{2\pi x}{\lambda}$$

How, $\Psi_{(x)}$ changes with time,
(take derivatives)

$$\Rightarrow \frac{d\Psi_{(x)}}{dx} = -2a \frac{2\pi}{\lambda} \cdot \sin \frac{2\pi x}{\lambda}$$

rate of change (2nd derivative)

$$\Rightarrow \frac{d^2\Psi_{(x)}}{dx^2} = -2a \frac{4\pi^2}{\lambda^2} \cdot \cos \frac{2\pi x}{\lambda}$$

we can write,

$$\Rightarrow \frac{d^2\Psi_{(x)}}{dx^2} = -\frac{4\pi^2}{\lambda^2} \cdot \Psi_{(x)} = -\left(\frac{2\pi}{\lambda}\right)^2 \cdot \Psi_{(x)}$$





Schrödinger Wave Equation

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$$\Rightarrow \frac{d^2\Psi_{(x)}}{dx^2} = -\frac{4\pi^2}{\lambda^2} \cdot \Psi_{(x)} = -\left(\frac{2\pi}{\lambda}\right)^2 \cdot \Psi_{(x)}$$

from, de - Broglie eqn we know, $\lambda = \frac{h}{mv} = \frac{h}{p}$

$$\Rightarrow \frac{d^2\Psi_{(x)}}{dx^2} = -\frac{p^2}{\hbar^2} \cdot (\Psi_{(x)}). \quad \left[\text{where, } \hbar = \frac{h}{2\pi} \right]$$





Schrödinger Wave Equation

$$[T.E(E) = K.E + P.E]$$

$$\Rightarrow E = \frac{p^2}{2m} + v_{(x)}$$

$$\Rightarrow p^2 = 2m(E - v_{(x)})$$

$$\Rightarrow \frac{d^2\Psi_{(x)}}{dx^2} = -\frac{2m(E - v_{(x)})}{\hbar^2} \cdot (\Psi_{(x)})$$





Schrödinger Wave Equation

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$$\Rightarrow \frac{d^2 \Psi_{(x)}}{dx^2} = -\frac{2m(E - v_{(x)})}{\hbar^2} \cdot (\Psi_{(x)})$$

$$\Rightarrow -\frac{\hbar^2}{2m} \frac{d^2 \Psi_{(x)}}{dx^2} + v_{(x)} (\Psi_{(x)}) = E \cdot \Psi_{(x)}$$

$$\Rightarrow \underbrace{\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + v_{(x)} \right)}_{\hat{H} \text{ operator}} (\Psi_{(x)}) = E \cdot \Psi_{(x)}$$

$$\Rightarrow \hat{H} \Psi_{(x)} = E \cdot \Psi_{(x)}$$





Schrödinger Wave Equation

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$$\Rightarrow \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + v_{(x)} \right) (\Psi_{(x)}) = E \cdot \Psi_{(x)}$$

$$\Rightarrow \frac{d^2 \Psi_{(x)}}{dx^2} + \frac{8\pi^2 m}{h^2} (E - v_{(x)}) (\Psi_{(x)}) = 0$$

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} + \frac{8\pi^2 m}{h^2} (E - v) \Psi = 0$$





Q. The Correct Schrodinger's wave equation for a electron with total energy E and potential energy V is given by

(a)
$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} + \frac{8\pi^2}{mh^2} (E - V) \Psi = 0$$

(b)
$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} + \frac{8\pi m}{h^2} (E - V) \Psi = 0$$

(c)
$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} + \frac{8\pi^2 m}{h^2} (E - V) \Psi = 0$$

(d) None





Q. Wave mechanical model of the atom depends upon

(a) De-Broglie concept of dual nature of electron

(b) Heisenberg uncertainty principle

(c) Schrodinger uncertainty principle

(d) All





s Orbitals – Radial Part

n	ℓ	$R(r)$
1	0	$2\left(\frac{Z}{a_0}\right)^{3/2} e^{-\frac{Z}{a_0}r}$
2	0	$\left(\frac{1}{2\sqrt{2}}\right)\left(\frac{Z}{a_0}\right)^{3/2} \left(2 - \frac{Z}{a_0}r\right) e^{-\frac{Z}{2a_0}r}$
3	0	$\left(\frac{2}{81\sqrt{3}}\right)\left(\frac{Z}{a_0}\right)^{3/2} \left(27 - \frac{18Z}{a_0}r + \frac{2Z^2}{a_0^2}r^2\right) e^{-\frac{Z}{3a_0}r}$





p Orbitals – Radial Part

n	ℓ	$R(r)$
2	1	$\left(\frac{1}{2\sqrt{6}}\right)\left(\frac{Z}{a_0}\right)^{3/2} \frac{Z}{a_0} r e^{-\frac{Z}{2a_0}r}$
3	1	$\left(\frac{4}{81\sqrt{6}}\right)\left(\frac{Z}{a_0}\right)^{3/2} \left(\frac{6Z}{a_0}r - \frac{Z^2}{a_0^2}r^2\right) e^{-\frac{Z}{3a_0}r}$





Nodes:

Radial Nodes: $n - l - 1$

Angular nodes: l

Total Nodes: $n - 1$





Q. The Schrodinger wave equation for hydrogen atom is

$$\Psi_{2s} = \frac{1}{4(2\pi)^{1/2}} \left(\frac{1}{a_o} \right)^{3/2} \left(2 - \frac{r}{a_o} \right) e^{-r/2a_o}$$

Where, a_o is Bohr's radius. Let the radial node in 2s be at r_o . Then find r in terms of a_o

[IIT 2004]





Q. The Schrodinger wave equation for hydrogen atom is

$$\Psi(\text{radial}) = \frac{1}{16(4)^{1/2}} \left(\frac{z}{a_0} \right)^{3/2} ((\sigma - 1)(\sigma^2 - 8\sigma + 12)) e^{-\sigma/2}$$

Where, a_0 and z are the constant in which answer can be expressed and $\sigma = \frac{2zr}{a_0}$ minimum and maximum position of radial nodes from nucleus are respectively.

a. $\frac{a_0}{z}, \frac{3a_0}{z}$

b. $\frac{a_0}{2z}, \frac{a_0}{z}$

c. $\frac{a_0}{2z}, \frac{3a_0}{z}$

d. $\frac{a_0}{2z}, \frac{4a_0}{z}$





Q. Which of the following orbitals have two spherical nodes.

(a) 2s

(b) 4s

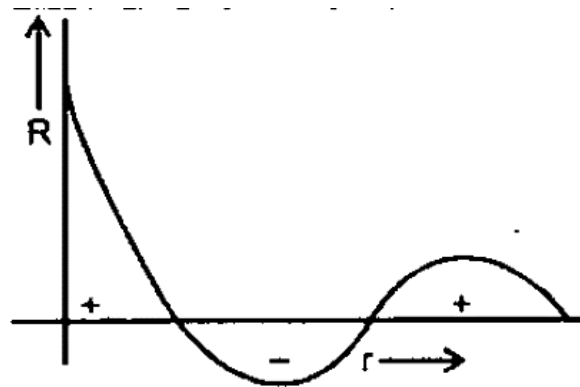
(c) 3d

(d) 6f





Q. Wave function of an orbital is plotted against the distance from nucleus. The graphical representation is of:



- (a) 1s
- (b) 2s
- (c) 3s
- (d) 2p

